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Generalised Point Interactions for the Radial Schrödinger Equation via Unitary Dilations

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Abstract

We present an inverse scattering construction of generalised point interactions (GPI) – point-like objects with non-trivial scattering behaviour. The construction is developed for single centre S-wave GPI models with rational S-matrices, and starts from an integral transform suggested by the scattering data. The theory of unitary dilations is then applied to construct a unitary mapping between Pontryagin spaces which extend the usual position and momentum Hilbert spaces. The GPI Hamiltonian is defined as a multiplication operator on the momentum Pontryagin space and its free parameters are fixed by a physical locality requirement. We determine the spectral properties and domain of the Hamiltonian in general, and construct the resolvent and Møller wave operators thus verifying that the Hamiltonian exhibits the required scattering behaviour. The physical Hilbert space is identified. The construction is illustrated by GPI models representing the effective range approximation. For negative effective range we recover a known class of GPI models, whilst the positive effective range models appear to be new. We discuss the interpretation of these models, along with possible extensions to our construction.

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1 Introduction and Main Ideas

Generalised point interactions (GPI) are solvable models in quantum mechanics representing point objects with non-trivial scattering behaviour. The prototype for such models is the class of point interactions (PI), corresponding to Hamiltonians with δ-function potentials essentially introduced by Fermi [1] and rigorously defined as self-adjoint extensions of $-\triangle$ on the domain of smooth functions compactly supported away from the interaction centre [2]. This construction leads to 1-parameter families of PI Hamiltonians in dimensions 2 and 3 which provide the leading order (scattering length) approximation to the scattering behaviour of Schrödinger operators with short range potentials in the sector of zero angular momentum (see, for example [3]). We refer to [4] for an extensive bibliography on PI models.

GPI models are employed to treat more general scattering behaviour, such as higher order corrections to S-wave scattering, non-trivial scattering in non-zero angular momentum sectors or point objects in dimensions $d \geq 4$. Such models have been studied for a long time from the pseudo-potential viewpoint in many body physics – see [5, 6]. The mathematical study of such generalised point interaction (GPI) models began in the Russian literature with the work of Shirokov [7], and more rigorous formulations were later developed by Pavlov [8, 9, 10] and Shondin [11, 12] (see also [13]). In contrast to PI models, GPI Hamiltonians are not defined on the usual Hilbert space $L^2(\mathbb{R}^d)$, but on an extended space whose inner product may be indefinite, in which case one must identify a physical Hilbert space of states in order to recover the probability interpretation of quantum mechanics.

In this paper, we introduce and develop a new inverse scattering construction for single centre GPI models with non-trivial S-wave scattering. It is currently an open problem to extend this construction to higher angular momenta and dimensions $d \geq 4$; we discuss this further in the Conclusion. Our method is based on the technique of *unitary dilations* due in origin to Sz.-Nagy [14] and extended by Davis [15].

The S-wave inverse scattering problem has been partially studied by Shondin [11], as we describe below. First, let us briefly mention the two principal non-inverse GPI constructions, which we call the *auxiliary space* and *distributional* methods. In the auxiliary space method, developed by Pavlov and co-workers [9, 10], one starts with a given extended Hilbert space and then seeks the class of GPI Hamiltonians which 'live' on this space. On the other hand, the distributional method of Shondin [12] is a direct attempt to define $H = -\triangle + |\omega\rangle\langle\omega|$, where ω is somewhere in the $j < 0$ portion of the scale of Sobolev spaces $\mathcal{H}_j = (-\triangle + 1)^{-j/2} L^2(\mathbb{R}^d)$. The construction leads to a Pontryagin space[1] $\Pi_m = \mathcal{H}_0 \oplus \mathbb{C}^{2m}$, where m is the unique integer such that $\omega \in \mathcal{H}_{-m-2} \backslash \mathcal{H}_{-m-1}$ and the inner product has signature (m, m) on the finite dimensional part. The GPI Hamiltonian is then defined on Π_m using Krein's formula [16].

Returning to the inverse problem, Shondin [11] considered the inverse scattering

[1] A Pontryagin space is an indefinite (Krein) inner product space with a finite rank of indefiniteness – see Section 2.1.

problem in $d = 3$ for S-wave scattering data of form

$$\cot \delta_0(k) = k^{-1} r(k^2), \tag{1.1}$$

where $r(z)$ is a rational function with real coefficients. Shondin refers to this class of data as the 'R class': it corresponds exactly with the class of rational S-wave S-matrices satisfying the usual analytic continuation property $S(k) = S^*(-k)$ [17]. In particular, the R class contains truncated low energy expansions of form

$$\cot \delta_0(k) = -\frac{1}{kL} + \frac{1}{2} k r_0 + k^3 r_1 + \cdots + k^{2n+1} r_n, \tag{1.2}$$

for low energy parameters $L, r_0, r_1, \ldots, r_n$ and any $n \geq 0$, and thus furnishes approximations to the low energy S-wave behaviour of Schrödinger operators with short range potentials to arbitrary order. Shondin's method starts by writing down a candidate resolvent on a (positive definite) extension of the usual Hilbert space. (In this respect it resembles the auxiliary space method). Various free functions in this resolvent are then fixed by requiring that the candidate be the resolvent of a self-adjoint operator. However, this method is limited to those $r(z)$ with negative imaginary part in the upper half plane, which is a somewhat restrictive sub-class: for example, scattering data of form (1.2) is possible only with $r_1, \ldots, r_n = 0$ and $r_0 < 0$. As we will see later, in the context of our method, more general scattering data corresponds to GPI models defined on Pontryagin spaces. Thus, in order to apply Shondin's method to such data, one would have to guess not only the appropriate extension to the Hilbert space, but also its inner product, thereby rendering it much less practical as a construction.

In contrast, the method proposed here allows one to treat the full R class. It proceeds from the simple observation that, for point-like interactions, the scattering data $\delta_0(k)$ completely specify the S-wave continuum eigenfunctions as $u_k(r) = (2/\pi)^{1/2} \sin(kr + \delta_0(k))$, when scattering normalisation is imposed. This is quite different from the usual situation in inverse scattering theory, where the scattering data specifies (in the first instance) only the asymptotic form of the $u_k(r)$. As a result, the inverse scattering problem for GPI models can be solved without recourse to the usual Gel'fand-Levitan machinery.

The $u_k(r)$ define an integral transform $\mathcal{T}$ between $\mathcal{H}_r = L^2((0,\infty), dr)$ and $\mathcal{H}_k = L^2((0,\infty), dk)$, (i.e., the radial position and momentum Hilbert spaces) by

$$(\mathcal{T}\psi)(k) = \left(\frac{2}{\pi}\right)^{1/2} \int_0^\infty \sin(kr + \delta_0(k)) \psi(r) dr, \tag{1.3}$$

We adopt $\mathcal{T}$ as a candidate for an eigenfunction transform associated with our desired GPI Hamiltonian h_{gpi}. Of course, $\mathcal{T}$ cannot be the full eigenfunction transform unless it is unitary, in which case we can define $h_{\text{gpi}} = \mathcal{T}^* k^2 \mathcal{T}$. However, when $\mathcal{T}$ is non-unitary, we may 'dilate' it to a unitary operator between enlarged inner product spaces, using the theory of unitary dilations as follows. Firstly, we quantify the departure of $\mathcal{T}$ from unitarity by the operators $M_1 = \mathbb{1} - \mathcal{T}\mathcal{T}^*$ and $M_2 = \mathbb{1} - \mathcal{T}^*\mathcal{T}$, and the closures $\mathcal{M}_1$ and

$\mathcal{M}_2$ of their respective ranges. For scattering data in the R class, we will show that the rank and signature of M_1 and M_2 are finite and given in terms of indices reminiscent of Levinson's theorem [17].

Next, we define indefinite inner products on the $\mathcal{M}_i$, together with an operator $\hat{\mathcal{T}} : \mathcal{H}_r \oplus \mathcal{M}_1 \to \mathcal{H}_k \oplus \mathcal{M}_2$ which is unitary with respect to the relevant inner products and satisfies $P_{\mathcal{H}_k}\hat{\mathcal{T}}|_{\mathcal{H}_r} = \mathcal{T}$, where $P_{\mathcal{H}_k}$ is the orthoprojector onto $\mathcal{H}_k$. $\hat{\mathcal{T}}$ is said to be a unitary dilation[2] of $\mathcal{T}$. We emphasise that the construction of $\hat{\mathcal{T}}$ and the enlarged inner product spaces requires no information beyond that encoded in $\mathcal{T}$, and is unique up to a unitary equivalence and further dilation. To complete the construction, we define the GPI Hamiltonian $h_{\rm gpi}$ by

$$h_{\rm gpi} = \hat{\mathcal{T}}^\dagger \begin{pmatrix} k^2 & 0 \\ 0 & \Lambda \end{pmatrix} \hat{\mathcal{T}}, \tag{1.4}$$

where the dagger denotes the Pontryagin space adjoint, and we have used an obvious block matrix notation. We will show that Λ is completely determined by imposing a physical locality requirement: that the 'interaction' be localised at the origin. Mathematically, this is expressed by requiring the Hamiltonian agrees with the free Hamiltonian away from the interaction centre, i.e., $h_{\rm gpi}(\psi, 0)^T = (-\psi'', 0)^T$ if $\psi \in C_0^\infty(0, \infty)$. Subject to this locality condition, we have thus constructed both $h_{\rm gpi}$ and its spectral representation. The non-uniqueness in our construction leads to a family of unitarily equivalent GPI Hamiltonians with the same spectral and scattering properties.

Our plan is as follows. In Section 2, we briefly describe some features of analysis in indefinite inner product spaces, and also describe the construction of unitary dilations, essentially following Davis [15]. In addition, we sketch our construction in a more abstract setting. Next, in Section 3, we explicitly construct the operators M_1 and M_2 (which are of finite rank) for a generic subclass of the R class – those whose scattering amplitudes exhibit only simple poles on the physical sheet – and compute their rank and signature. In Section 4, we construct $h_{\rm gpi}$ as described above. Subject to the locality condition, we show that the eigenvalues of $h_{\rm gpi}$ occur at precisely those energies for which the scattering amplitude derived from (1.1) exhibits poles on the physical sheet, as is the case for ordinary scattering from 'nice' potentials. We construct the corresponding eigenfunctions of $h_{\rm gpi}$, and isolate the physical Hilbert space. We also determine the domain and resolvent of $h_{\rm gpi}$, and explicitly construct its Møller wave operators in a two-space setting, verifying that they exhibit the required scattering theory.

In Section 5, we illustrate our procedure by constructing GPI models with scattering behaviour $\cot\delta_0(k) = -1/(kL) + kM$, representing the effective range approximation of low energy scattering theory [17]. In the case $M < 0$, $\mathcal{H}_r$ and $\mathcal{H}_k$ are extended to larger Hilbert spaces, and we recover the models of 'type B_2' previously constructed by Shondin [11]. These models also arise as a special case of the auxiliary space construction in [8]. The case $M > 0$, for which Pontryagin spaces are required, appears to be new. Our methods allow the entire class of GPI Hamiltonians to be constructed, along with their spectral representations. A particularly interesting subclass of the models constructed

[2]See Section 2 for a note on the nomenclature.

corresponds to the case $L = \infty$, with scattering theory $\cot \delta_0(k) = kM$. Such models reproduce the leading order behaviour of non-point interactions exhibiting a zero energy resonance. We refer to these models as *resonance point interactions* (RPI).

We also discuss how these GPI models may be used as models for Schrödinger operators with spherically symmetric potentials of compact support. To do this, we employ a general methodology for discussing the 'large scale effects of small objects' developed by Kay and the author [3]. In particular, we develop *fitting formulae* (analogous to those given in [3]) for matching a given potential $V(r)$ to the 'best fit' GPI model. Finally, in Section 6, we conclude by discussing various extensions to our method.

The motivation for the present work arose in a consideration of the scattering of charged particles off magnetic flux tubes of small radius [18], in which it was found that the scattering lengths for spin-$\frac{1}{2}$ particles generically take the values 0 or ∞ in certain angular momentum sectors. In consequence, the analogue of PI models representing dynamics in the background of an infinitesimally thin wire of flux fails to describe the leading order scattering theory in these sectors, and should be replaced by models analogous to the RPI models mentioned above. The special nature of this system can be attributed to the fact that it is an example of supersymmetric quantum mechanics. Elsewhere [19], we will construct the appropriate class of RPI for this system.

2 Preliminaries

2.1 Unitary Dilations

We begin by describing the unitary dilation theory required in the sequel. Let $\mathcal{H}_1, \ldots, \mathcal{H}_4$ be Hilbert spaces and $T \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$. Then $\hat{T} \in \mathcal{L}(\mathcal{H}_1 \oplus \mathcal{H}_3, \mathcal{H}_2 \oplus \mathcal{H}_4)$ is called a *dilation* of T if $T = P_{\mathcal{H}_2} \hat{T}|_{\mathcal{H}_1}$ where $P_{\mathcal{H}_2}$ is the orthogonal projector onto $\mathcal{H}_2$. In block matrix form, $\hat{T}$ takes form

$$\hat{T} = \begin{pmatrix} T & P \\ Q & R \end{pmatrix}. \tag{2.1}$$

Our nomenclature follows that of Halmos [20]. Elsewhere (e.g., in the work of Davis [15]), the term 'dilation' (or 'dilatation') often means that $\hat{T}^n$ is a dilation of T^n and $(\hat{T}^*)^n$ is a dilation of $(T^*)^n$ for each $n = 1, 2, \ldots$ (in addition, $\mathcal{H}_1 = \mathcal{H}_2$, and $\mathcal{H}_3 = \mathcal{H}_4$). We refer to such operators as *power dilations*: in the block form (2.1), this requires $PR^nQ = 0$ for each $n = 0, 1, 2, \ldots$.

According to a result of Sz.-Nagy [14], any contraction T from one Hilbert space to another (i.e., a bounded operator satisfying $\|T\| \leq 1$) has a unitary dilation between larger Hilbert spaces. Subsequently, Davis [15] extended this result to arbitrary closed densely defined operators at the cost of introducing indefinite inner product spaces. (It is clear that if $\|T\| > 1$, no Hilbert space unitary dilation is possible.) In fact, Davis' construction yields a unitary *power* dilation of the original operator. This has no physical relevance in our construction, and so we use a more economical 'cut-down' version of

Davis' result, described below. First, we briefly review the salient features of analysis in indefinite inner product spaces. Full treatments can be found in the monographs of Bognár [21] and Azizov and Iokhvidov [22].

We employ a particular class of indefinite inner product spaces known as *J-spaces*. Let $\mathcal{H}$ be a Hilbert space with (positive definite) inner product $\langle \cdot \mid \cdot \rangle$, equipped with a unitary involution, J. We define a non-degenerate indefinite inner product $[\cdot, \cdot]$ on $\mathcal{H}$ by

$$[x, y] = \langle x \mid Jy \rangle, \tag{2.2}$$

which we call the *J-inner product*. $\mathcal{H}$ equipped with the J-inner product is called a J-space. $\mathcal{H}$ admits decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_- = \mathcal{H}_+[+]\mathcal{H}_-$ into the eigenspaces $\mathcal{H}_\pm$ of J with eigenvalue ± 1, where $[+]$ denotes the orthogonal direct sum in the J-inner product. If at least one of the $\mathcal{H}_\pm$ is finite dimensional, then $\mathcal{H}$ is a *Pontryagin space* with respect to $[\cdot, \cdot]$.

The topology of a J-space is determined by the Hilbert space norm; however, operator adjoints and the notion of unitarity are defined relative to the J-inner product. Thus if $\mathcal{H}_i$ $(i = 1, 2)$ are J_i-spaces, and $T \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$, the (J_1, J_2)-*adjoint* $T^\dagger$ of T is defined in terms of the Hilbert space adjoint T^* by

$$T^\dagger = J_1 T^* J_2. \tag{2.3}$$

Equivalently, $[T^\dagger x, y]_{\mathcal{H}_1} = [x, Ty]_{\mathcal{H}_2}$ for all $x \in \mathcal{H}_2$, $y \in \mathcal{H}_1$. If $[Ux, Uy]_{\mathcal{H}_2} = [x, y]_{\mathcal{H}_1}$ for all $x, y \in \mathcal{D} \subset \mathcal{H}_1$, U is said to be (J_1, J_2)-*isometric*; if in addition U is a linear isomorphism of $\mathcal{H}_1$ and $\mathcal{H}_2$, and $\mathcal{D} = \mathcal{H}_1$, U is said to be (J_1, J_2)-*unitary*. Equivalently, $UU^\dagger = \mathbb{1}_{\mathcal{H}_1}$ and $U^\dagger U = \mathbb{1}_{\mathcal{H}_2}$. If $\mathcal{H}_1 = \mathcal{H}_2$ with $J_1 = J_2 = J$, terms such as (J_1, J_2)-isometric are abbreviated to J-isometric etc.

Returning to the construction of unitary dilations, let T be any bounded operator $T \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$, and define operators $M_1 = \mathbb{1} - TT^*$ and $M_2 = \mathbb{1} - T^*T$. It is trivial to show that the respective closures $\mathcal{M}_i = \overline{\operatorname{Ran} M_i}$ of their ranges are $\operatorname{sgn}(M_i)$-spaces, and hence that $\mathcal{K}_i = \mathcal{H}_i \oplus \mathcal{M}_i$ are J_i-spaces, where $J_i = \mathbb{1}_{\mathcal{H}_i} \oplus \operatorname{sgn}(M_i)$. We now define a dilation $\hat{T}$ of T by

$$\hat{T} = \begin{pmatrix} T & -\operatorname{sgn}(M_1)|M_1|^{1/2} \\ |M_2|^{1/2} & T^*|_{\mathcal{M}_1} \end{pmatrix}, \tag{2.4}$$

which has (J_1, J_2)-adjoint $\hat{T}^\dagger$ equal to

$$\hat{T}^\dagger = J_1 \hat{T}^* J_2 = \begin{pmatrix} T^* & \operatorname{sgn}(M_2)|M_2|^{1/2} \\ -|M_1|^{1/2} & T|_{\mathcal{M}_2} \end{pmatrix}. \tag{2.5}$$

Here, we have used the intertwining relations $Tf(T^*T) = f(TT^*)T$ and $T^*f(TT^*) = f(T^*T)T^*$, which hold for any continuous Borel function f. It is now easy to show that $\hat{T}^\dagger \hat{T} = \mathbb{1}_{\mathcal{K}_1}$ and $\hat{T}\hat{T}^\dagger = \mathbb{1}_{\mathcal{K}_2}$, thus verifying that $\hat{T}$ is a (J_1, J_2)-unitary dilation of T. In our application, M_1 and M_2 are finite rank, and so the J-spaces constructed above are Pontryagin spaces.

We briefly consider the uniqueness of the unitary dilations constructed above. Suppose $\mathcal{N}_i$ are J_i spaces ($i = 1, 2$) and that $\tilde{T} : \mathcal{H}_1 \oplus \mathcal{N}_1 \to \mathcal{H}_2 \oplus \mathcal{N}_2$ is a unitary dilation of T with matrix form (2.1). Then, provided that the M_i are finite rank, one may show that

$$P_{\mathcal{H}_2 \oplus \mathcal{Q}} \tilde{T}|_{\mathcal{H}_1 \oplus \mathcal{P}} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & U_2 \end{pmatrix} \hat{T} \begin{pmatrix} \mathbb{1} & 0 \\ 0 & U_1^\dagger \end{pmatrix}, \tag{2.6}$$

where $\mathcal{P} = P^\dagger \overline{\mathrm{Ran}\, M_1}$, $\mathcal{Q} = Q \overline{\mathrm{Ran}\, M_1}$, and U_1 and U_2 are unitaries (with respect to the J-inner products) from $\mathcal{M}_1$ and $\mathcal{M}_2$ to $\mathcal{P}$ and $\mathcal{Q}$ respectively. In addition, $P_{\mathcal{H}_2 \oplus \mathcal{Q}}$ is an orthogonal projection onto $\mathcal{H}_2 \oplus \mathcal{Q}$ in $\mathcal{H}_2 \oplus \mathcal{N}_2$.

Thus $\hat{T}$ is unique up to further dilation and unitary equivalence of the above form. If the M_i are not of finite rank, this statement also holds if the M_i are strictly positive. More generally, it is not clear whether $\mathcal{Q}$ is necessarily orthocomplemented, and therefore whether $P_{\mathcal{H}_2 \oplus \mathcal{Q}}$ exists.

2.2 Abstract Setting

In this section, we sketch our construction in a general setting, which makes clear how it may be extended. In particular, we show how the domain and action of the Hamiltonian is determined.

Let $\mathcal{H}_i$ ($i = 1, 2$) be Hilbert spaces and let A be a densely defined symmetric operator with domain $\mathcal{D} \subset \mathcal{H}_1$. Suppose that A possesses two self-adjoint extensions $A_\pm$ such that

$$A_\pm = \mathcal{T}_\pm^* \tilde{A} \mathcal{T}_\pm \tag{2.7}$$

where $\tilde{A}$ is a self-adjoint operator on $\mathcal{H}_2$ with $(\tilde{A} + \omega)^{-1}$ bounded for some $\omega \in \mathbb{R}$, and $\mathcal{T}_\pm$ are unitary operators $\mathcal{T}_\pm : \mathcal{H}_1 \to \mathcal{H}_2$. Let a_+ and a_- be bounded operators on $\mathcal{H}_2$ which commute with $\tilde{A}$ and define

$$\mathcal{T} = a_+ \mathcal{T}_+ + a_- \mathcal{T}_-. \tag{2.8}$$

In our application, $a_\pm$ are determined by the scattering data. We define M_1 and M_2 as above, for simplicity assuming that they are finite rank (as they are in our application). The unitary dilation $\hat{\mathcal{T}}$ derived above is then used to define a self-adjoint operator B on the Pontryagin space $\Pi_1 = \mathcal{H}_1 \oplus \mathcal{M}_1$ by

$$B = \hat{\mathcal{T}}^\dagger \begin{pmatrix} \tilde{A} & 0 \\ 0 & \Lambda \end{pmatrix} \hat{\mathcal{T}}, \tag{2.9}$$

where Λ is a self-adjoint operator on $\mathcal{M}_2$ (with respect to its inner product). Thus

$$B \begin{pmatrix} \varphi \\ \Phi \end{pmatrix} = \begin{pmatrix} \mathcal{T}^* \tilde{A}(\mathcal{T}\varphi - \Theta) + \operatorname{sgn} M_2 |M_2|^{1/2} \Lambda(|M_2|^{1/2}\varphi + \mathcal{T}^*|_{\mathcal{M}_1}\Phi) \\ -|M_1|^{1/2} \tilde{A}(\mathcal{T}\varphi - \Theta) + \mathcal{T}|_{\mathcal{M}_2} \Lambda(|M_2|^{1/2}\varphi + \mathcal{T}^*|_{\mathcal{M}_1}\Phi) \end{pmatrix}, \tag{2.10}$$

where $\Theta = \operatorname{sgn} M_1 |M_1|^{1/2}\Phi$ (considered as an element of $\mathcal{H}_2$), and B has domain

$$D(B) = \{(\varphi, \Phi)^T \mid \mathcal{T}\varphi - \Theta \in D(\tilde{A})\}. \tag{2.11}$$

To gain a more explicit description of $D(B)$, we impose the requirement that B be a self-adjoint extension of the *non-densely defined* operator $A \oplus 0$ on $\mathcal{D} \oplus 0 \subset \Pi_1$, i.e., $B(\varphi, 0)^T = (A\varphi, 0)^T$ for all $\varphi \in \mathcal{D}$. Later this will carry the physical interpretation of a locality condition. It is easy to show that this requirement is satisfied if and only if $\mathcal{M}_2$ is invariant under A^* and

$$\Lambda = (|M_2|^{-1/2} A^*|_{\mathcal{M}_2} |M_2|^{1/2})^*. \tag{2.12}$$

As a consequence of locality, we note that if $(\varphi, \Phi)^T \in D(B)$ with $B(\varphi, \Phi)^T = (\tilde{\varphi}, \tilde{\Phi})^T$, then $\varphi \in D(A^*)$, and $\tilde{\varphi} = A^*\varphi$. For take any $\psi \in \mathcal{D}$. Then

$$\langle \tilde{\varphi} \mid \psi \rangle_{\mathcal{H}_1} = \left[\begin{pmatrix} \tilde{\varphi} \\ \tilde{\Phi} \end{pmatrix}, \begin{pmatrix} \psi \\ 0 \end{pmatrix} \right]_{\Pi_1} = \left[\begin{pmatrix} \varphi \\ \Phi \end{pmatrix}, B \begin{pmatrix} \psi \\ 0 \end{pmatrix} \right]_{\Pi_1} = \langle \varphi \mid A\psi \rangle_{\mathcal{H}_1}. \tag{2.13}$$

We may therefore re-write (2.11) as

$$D(B) = \left\{ \begin{pmatrix} \varphi \\ \Phi \end{pmatrix} \mid \varphi \in D(A^*), \quad \Theta_1 \in D(\tilde{A}) \right\}, \tag{2.14}$$

where $\Theta_1 = a_+\mathcal{T}_+\chi_+ + a_-\mathcal{T}_-\chi_- + \Theta$ and $\chi_\pm = (A_\pm + \omega)^{-1}(A^* + \omega)\varphi - \varphi$. The advantage of this expression is that $\chi_\pm$ can be shown to be the unique element of $\ker(A^* + \omega)$ such that $\varphi + \chi_\pm \in D(A_\pm)$. In our application, $\chi_\pm$ may be expressed in terms of the value of φ and its first derivative at the origin.

To determine the action of B more explicitly, we use the fact that the upper component of the right-hand side of (2.10) is equal to $A^*\varphi$ in order to compute $\tilde{\Theta} = \operatorname{sgn} M_1 |M_1|^{1/2}\tilde{\Phi}$. We obtain

$$\tilde{\Theta} = -M_1\tilde{A}(\mathcal{T}\varphi - \Theta) + \mathcal{T}(A^*\varphi - \mathcal{T}^*\tilde{A}(\mathcal{T}\varphi - \Theta)) = \mathcal{T}A^*\varphi - \tilde{A}(\mathcal{T}\varphi - \Theta) \tag{2.15}$$

Using the fact that $\Theta_1 \in D(\tilde{A})$, this becomes

$$\tilde{\Theta} = \tilde{A}\Theta_1 + \omega(\Theta_1 - \Theta) + \mathcal{T}(A^* + \omega)\varphi - (\tilde{A} + \omega)(\mathcal{T}\varphi + \Theta_1 - \Theta). \tag{2.16}$$

The last two terms cancel by definition of $\chi_\pm$ and we conclude that

$$B \begin{pmatrix} \varphi \\ \Phi \end{pmatrix} = \begin{pmatrix} A^*\varphi \\ (\operatorname{sgn} M_1 |M_1|^{1/2})^{-1}\tilde{\Theta} \end{pmatrix} \tag{2.17}$$

where $\tilde{\Theta} = \tilde{A}\Theta_1 + \omega(a_+\mathcal{T}_+\chi_+ + a_-\mathcal{T}_-\chi_-)$.

3 Determination of M_1 and M_2

In this section, we determine the operators $M_1 = \mathbb{1} - \mathcal{T}\mathcal{T}^*$ and $M_2 = \mathbb{1} - \mathcal{T}^*\mathcal{T}$, where $\mathcal{T}$ is an integral transformation arising from the scattering data in the Shondin R class [11] given by

$$\cot\delta_0(k) = k^{-1}\frac{p(k^2)}{q(k^2)}, \qquad \delta_\ell(k) \equiv 0 \quad \text{for } \ell \geq 1, \tag{3.1}$$

where $p(z)$ and $q(z)$ are coprime polynomials in $\mathbb{R}[z]$, the ring of polynomials with real coefficients. In particular, we will show how the rank and signature of the M_i are determined by two 'Levinson indices' defined below. We emphasise that our methods are very different to those of Shondin.

The scattering amplitude corresponding to $\delta_0(k)$ is

$$f_0(k) = \frac{1}{k}e^{i\delta_0(k)}\sin\delta_0(k) = \frac{q(k^2)}{p(k^2) - ikq(k^2)}. \tag{3.2}$$

Defining the polynomial $W(z)$ by

$$W(z) = \begin{cases} p(-z^2) - zq(-z^2) & p(0) \neq 0 \\ p(-z^2)/z - q(-z^2) & p(0) = 0, \end{cases} \tag{3.3}$$

we note that $f_0(k)$ exhibits poles where $W(ik) = 0$. The set Ω of zeros of $W(z)$ in the left-hand half-plane $\operatorname{Re} z < 0$ corresponds to poles of $f_0(k)$ such that k^2 lies on the physical sheet. We refer to the situation where these poles (and hence the corresponding zeros of $W(z)$) are simple as the *generic case*. In Theorem 4.1, we will show that the discrete spectrum of the GPI Hamiltonian is precisely $\{E = -\omega^2 \mid \omega \in \Omega\}$ under the requirement of locality.[3]

The qualitative features of the scattering data (3.1) are described by the degrees of p and q, two indices $I_L^\pm$ defined below, and the asymptotic behaviour of $\cot\delta_0(k)$ given by

$$\sigma_0 = \operatorname{sgn}\lim_{k\to 0^+}\cot\delta_0(k) \qquad \text{and} \qquad \sigma_\infty = \operatorname{sgn}\lim_{k\to\infty}\cot\delta_0(k), \tag{3.4}$$

where the limits are allowed to be $\pm\infty$. The indices $I_L^\pm$ are defined by

$$I_L^+ = \frac{\delta_0(0) - \delta_0(\infty)}{\pi} \qquad \text{and} \qquad I_L^- = \frac{\zeta(0) - \zeta(\infty)}{\pi}, \tag{3.5}$$

where the auxiliary scattering data $\zeta(k)$ is defined as a continuous function on $\mathbb{R}^+$ by

$$\cot\zeta(k) = -k^{-1}\frac{p(-k^2)}{q(-k^2)}. \tag{3.6}$$

We refer to $I_L^\pm$ as the Levinson indices (although Levinson's theorem [17] will not hold in its usual form).

[3] These eigenvalues can be complex: we will return to this point in section 5.3.

We now define the integral transform $\mathcal{T} = \cos\delta_0(k)\mathcal{S} + \sin\delta_0(k)\mathcal{C}$, which is suggested by the naïve generalised eigenfunctions $u_k(r) = (2/\pi)^{1/2}\sin(kr + \delta_0(k))$. Here, $\mathcal{S}$ and $\mathcal{C}$ are the sine and cosine transforms, defined by

$$(\mathcal{S}\psi)(k) = \sqrt{\frac{2}{\pi}}\int_0^\infty dr\,\psi(r)\sin kr \quad \text{and} \quad (\mathcal{C}\psi)(k) = \sqrt{\frac{2}{\pi}}\int_0^\infty dr\,\psi(r)\cos kr \tag{3.7}$$

(the integrals are intended as limits in L^2-norm). Both are unitary maps from $\mathcal{H}_r$ to $\mathcal{H}_k$; their inverses have the same form, with r and k exchanged. Thus $\mathcal{T}$ is given explicitly by

$$\mathcal{T} = \frac{p(k^2)}{(p(k^2)^2 + k^2q(k^2)^2)^{1/2}}\mathcal{S} + \frac{kq(k^2)}{(p(k^2)^2 + k^2q(k^2)^2)^{1/2}}\mathcal{C}. \tag{3.8}$$

Because $\mathcal{S}$ and $\mathcal{C}$ furnish the spectral representations of $-d^2/dr^2$ on $L^2(\mathbb{R}^+)$ with Dirichlet and Neumann boundary conditions respectively at the origin, we are in the general situation of Section 2.2.

We now restrict to the generic case and explicitly construct the M_i and compute their rank and signature. M_2 is given by the following proposition, whose proof is given later in this section.

Proposition 3.1 *In the generic case,*

$$M_2 = \sum_{\omega\in\Omega}\alpha_\omega|\xi_\omega\rangle\langle\xi_{\overline{\omega}}|, \tag{3.9}$$

where $\xi_\omega(r) = e^{\omega r}$*, and* α_ω *is the residue*

$$\alpha_\omega = \mathrm{Res}_\omega 2zf_0(-iz). \tag{3.10}$$

In addition, $\mathrm{Ran}\,M_2 = \mathrm{span}\,\{\xi_\omega \mid \omega\in\Omega\}$*, and*

$$\begin{aligned}\mathrm{rank}\,M_2 &= \frac{1}{2}\deg W + I_L^+ &(3.11)\\ \mathrm{sig}\,M_2 &= \frac{1}{2}\left(\sigma_0^2 - \sigma_\infty^2\right) - I_L^-. &(3.12)\end{aligned}$$

Next, define $\mathcal{M}_1$ to be the space of all L^2-vectors of form $Q(k^2)k(p(k^2)^2+k^2q(k^2)^2)^{-1/2}$, such that $Q(z)\in\mathbb{C}[z]$ is a polynomial with complex coefficients. Thus

$$\mathcal{M}_1 = (p(k^2)^2 + k^2q(k^2)^2)^{-1/2}k\mathbb{C}_{\mathfrak{V}-1}[k^2] \tag{3.13}$$

where $\mathbb{C}_r[z]$ is the $r+1$-dimensional complex vector space of polynomials with complex coefficients and degree at most r, and $\mathfrak{V} = \dim\mathcal{M}_1$ is given by

$$\mathfrak{V} = \frac{1}{2}\deg W + \frac{1}{2}(\sigma_\infty^2 - \sigma_0^2) = \max\{\deg p, \deg q\}. \tag{3.14}$$

M_1 is described by

Proposition 3.2 *In the generic case, M_1 vanishes on ${\mathcal{M}_1}^\perp$, and its action on $\mathcal{M}_1$ is given by $M_1 Q(k^2)k(p(k^2)^2 + k^2 q(k^2)^2)^{-1/2} = \tilde{Q}(k^2)k(p(k^2)^2 + k^2 q(k^2)^2)^{-1/2}$, where*

$$\tilde{Q}(k^2) = Q(k^2) + \sum_{\omega\in\Omega} \frac{Q(-\omega^2)\alpha_\omega}{q(-\omega^2)} \frac{p(k^2) - \omega q(k^2)}{\omega^2 + k^2}. \tag{3.15}$$

Moreover, $\operatorname{Ran} M_1 = \mathcal{M}_1$ *and*

$$\begin{aligned} \operatorname{rank} M_1 &= \frac{1}{2}\deg W + \frac{1}{2}(\sigma_\infty^2 - \sigma_0^2) && (3.16)\\ \operatorname{sig} M_1 &= -(I_L^+ + I_L^-). && (3.17) \end{aligned}$$

As an example, let us consider the sub-class of the R class considered by Shondin [11]; namely, the case where $r(z) = p(z)/q(z)$ has negative imaginary part in the upper half-plane. In this case, it is easy to show that there can be no solutions to $r(-z^2) = z$ and hence to $W(z) = 0$ in the left-hand half-plane, except on the real axis. Moreover, one can show that the residues α_ω at these zeros are necessarily positive, so M_2 is a positive operator as a result of (3.9). Accordingly, $\mathcal{T}$ is contractive, and our method yields a unitary dilation defined on Hilbert spaces. This explains why Shondin was able to construct these GPI models on enlarged *Hilbert* spaces.

We now prove the above propositions.

Proof of Proposition 3.1: M_2 may be written in two equivalent forms:

$$\begin{aligned} M_2 &= \mathcal{S}^{-1}\sin^2\delta_0(k)\mathcal{S} - \mathcal{C}^{-1}\sin^2\delta_0(k)\mathcal{C} \\ &\quad -\mathcal{C}^{-1}\sin\delta_0(k)\cos\delta_0(k)\mathcal{S} - \mathcal{S}^{-1}\sin\delta_0(k)\cos\delta_0(k)\mathcal{C} && (3.18)\\ &= \mathcal{C}^{-1}\cos^2\delta_0(k)\mathcal{C} - \mathcal{S}^{-1}\cos^2\delta_0(k)\mathcal{S} \\ &\quad -\mathcal{C}^{-1}\sin\delta_0(k)\cos\delta_0(k)\mathcal{S} - \mathcal{S}^{-1}\sin\delta_0(k)\cos\delta_0(k)\mathcal{C}. && (3.19) \end{aligned}$$

To convert this into an integral kernel we use the following Lemma, which may be proved by standard means (cf. Theorem IX.29 in [23]). Here, $v(x)$ and $w(x)$ stand for either $\sin x$ or $\cos x$, and $\mathcal{V}$ and $\mathcal{W}$ are the corresponding integral transforms from $\mathcal{H}_r$ to $\mathcal{H}_k$.

Lemma 3.3 *Let $g(k) \in L^2(\mathbb{R}^+) \cap L^\infty(\mathbb{R}^+)$ and define $G = \mathcal{V}^{-1}g(k)\mathcal{W}$. Then G has integral kernel*

$$G(r, r') = \frac{2}{\pi}\int_0^\infty v(kr)w(kr')g(k)dk, \tag{3.20}$$

(where the integral is a limit in L^2-norm).

In the case $\deg p > \deg q$, $\sin^2\delta_0(k)$ and $\sin\delta_0(k)\cos\delta_0(k)$ are $L^2 \cap L^\infty$ and so, applying Lemma 3.3 to (3.18) and combining terms, M_2 has integral kernel

$$M_2(r, r') = \frac{i}{\pi}\int_{-\infty}^\infty e^{i\delta_0(k)}\sin\delta_0(k)e^{ik(r+r')}dk = \frac{1}{\pi}\int_{-\infty}^\infty \frac{ikq(k^2)e^{ik(r+r')}}{p(k^2) - ikq(k^2)}dk. \tag{3.21}$$

Making the substitution $z = ik$ and closing the contour in the left-hand half-plane, the integrand has a simple pole at each $\omega \in \Omega$ and (3.9) follows. If $\deg q \geq \deg p$, we argue similarly using (3.19) to obtain the same result as before.

By linear independence of the ξ_ω and non-vanishing of the α_ω, it follows that $\operatorname{Ran} M_2 = \mathcal{M}_2 = \operatorname{span}\{\xi_\omega \mid \omega \in \Omega\}$, so $\operatorname{rank} M_2 = |\Omega|$, the cardinality of Ω. Using residue calculus, one may show that

$$|\Omega| = \frac{1}{2}\deg W + \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{W'(ik)}{W(ik)}dk. \tag{3.22}$$

By rewriting the second term as an integral over $(0,\infty)$, a small amount of algebra shows that the integrand is $-\pi^{-1}\delta_0'(k)$. Thus (3.11) is established.

To compute $\operatorname{sig} M_2$, we define the hermitian form $m_2(\varphi,\psi) : \mathcal{M}_2 \times \mathcal{M}_2 \to \mathbb{C}$ by $m_2(\varphi,\psi) = \langle \varphi \mid M_2\psi\rangle$. Labelling the elements of Ω as $\omega_1,\ldots,\omega_{|\Omega|}$, and writing $\psi = \sum_i c_i\xi_{\omega_i}$, we have

$$m_2(\psi,\psi) = \sum_{i,j,k} \overline{c_i}\langle\xi_{\omega_i} \mid \xi_{\omega_j}\rangle\alpha_j\langle\xi_{\overline{\omega_j}} \mid \xi_{\omega_k}\rangle c_k = c^\dagger\Xi^\dagger A\Xi c, \tag{3.23}$$

where A and Ξ are hermitian. Ξ has components $\Xi_{ij} = \langle\xi_{\omega_i} \mid \xi_{\omega_j}\rangle$, and is non-singular by linear independence of the ξ_ω. By Sylvester's Law of Inertia [24], the signature of M_2 equals that of A, which has components

$$A_{ij} = \begin{cases} \alpha_{\omega_i} & \omega_i = \overline{\omega_j} \\ 0 & \text{otherwise.} \end{cases} \tag{3.24}$$

A has eigenvalues $\{\alpha_\omega \mid \omega \in \mathbb{R}\} \cup \{\pm|\alpha_\omega| \mid \omega \notin \mathbb{R}\}$. Labelling the ω_i so that $\omega_1,\ldots,\omega_r$ are the real elements of Ω, we therefore have $\operatorname{sig} M_2 = \operatorname{sig}\operatorname{diag}(\alpha_{\omega_1}\ldots,\alpha_{\omega_r})$. (We have used the fact that $\alpha_{\overline{\omega}} = \overline{\alpha_\omega}$, and in particular that $\omega_r \in \mathbb{R}$ implies $\alpha_r \in \mathbb{R}$.) Defining $\zeta(k)$ by (3.6), it is easy to show that $\cot\zeta(-\omega) = 1$ for $\omega \in \Omega$, and that

$$\alpha_\omega = 2\lim_{z\to-\omega}\frac{z+\omega}{1-\cot\zeta(z)} = \frac{1}{\zeta'(-\omega)}. \tag{3.25}$$

Thus $\operatorname{sig}\operatorname{diag}(\alpha_1,\ldots,\alpha_r)$ is equal to the number of times that $\zeta(k) \equiv \pi/4 \pmod{\pi}$ as k traverses $\mathbb{R}^+$, counted according to the sign of $\zeta'(k)$ at such points. This is related to the Levinson index I_L^- by (3.12). ■

Proof of Proposition 3.2: We compute

$$\begin{aligned} M_1 \;=\; & -\frac{p(k^2)}{(p(k^2)^2+k^2q(k^2)^2)^{1/2}}\mathcal{S}\mathcal{C}^{-1}\frac{kq(k^2)}{(p(k^2)^2+k^2q(k^2)^2)^{1/2}} \\ & -\frac{kq(k^2)}{(p(k^2)^2+k^2q(k^2)^2)^{1/2}}\mathcal{C}\mathcal{S}^{-1}\frac{p(k^2)}{(p(k^2)^2+k^2q(k^2)^2)^{1/2}}, \end{aligned} \tag{3.26}$$

which vanishes identically on the closure of $\mathcal{D} = (p(k^2)^2+k^2q(k^2))^{1/2}\mathcal{S}C_0^\infty(0,\infty)$ as a result of elementary properties of the sine and cosine transforms. Furthermore, $\overline{\mathcal{D}}^\perp$ is

precisely the space $\mathcal{M}_1$ defined above, because $\psi \perp \mathcal{D}$ if and only if $(p(k^2)^2+k^2q(k^2))^{1/2}\psi$ is the sine transform of a distribution supported at the origin and therefore an odd polynomial (cf. Theorem V.11 in [25]). Hence M_1 vanishes on $\mathcal{M}_1^\perp$ and $\operatorname{Ran} M_1 \subset \mathcal{M}_1$.

Next, we compute the action of M_1 on $\mathcal{M}_1$. By contour integration,

$$\mathcal{T}^* \frac{kQ(k^2)}{(p(k^2)^2 + k^2q(k^2)^2)^{1/2}} = -\left(\frac{\pi}{2}\right)^{1/2} \sum_{\omega\in\Omega} \frac{Q(-\omega^2)\alpha_\omega}{q(-\omega^2)}\xi_\omega(r), \tag{3.27}$$

for polynomials $Q(z)$ such that the operand is in L^2. Moreover, it is easy to show that

$$T\xi_\omega = \left(\frac{2}{\pi}\right)^{1/2} \frac{k}{(p(k^2)^2 + k^2q(k^2)^2)^{1/2}} \frac{p(k^2) - \omega q(k^2)}{\omega^2 + k^2}, \tag{3.28}$$

from which the action of M_1 can be read off as required.

To compute the rank and signature of M_1, we use the fact that

$$\operatorname{rank} M_1 - \operatorname{rank} M_2 = \operatorname{sig} M_1 - \operatorname{sig} M_2 = \dim\ker \mathcal{T}^* - \dim\ker \mathcal{T}, \tag{3.29}$$

which follows from the intertwining relations $M_1\mathcal{T} = \mathcal{T}M_2$ and $M_2\mathcal{T}^* = \mathcal{T}^*M_1$. It therefore remains to determine the dimensions of the relevant kernels. Firstly, note that $\ker \mathcal{T}^* \subset \mathcal{M}_1$ and that (from (3.27)) $\psi = Q(k^2)k(p(k^2)^2 + k^2q(k^2)^2)^{-1/2} \in \ker \mathcal{T}^*$ if and only if $\psi \in \mathcal{M}_1$ and $Q(-\omega^2) = 0$ for each $\omega \in \Omega$. Thus $\prod_{\omega\in\Omega}(z + \omega^2)$ divides $Q(z)$ and so

$$\dim\ker \mathcal{T}^* = \min\{\mho - |\Omega|, 0\}. \tag{3.30}$$

Now consider $\ker \mathcal{T}$. We note that (3.28) may be rewritten

$$q(-\omega_i^2)\mathcal{T}\xi_{\omega_i} = \left(\frac{2}{\pi}\right)^{1/2} \frac{k}{(p(k^2)^2 + k^2q(k^2)^2)^{1/2}} \frac{p(k^2)q(-\omega_i^2) - p(-\omega_i^2)q(k^2)}{k^2 + \omega_i^2}, \tag{3.31}$$

and apply the following abstract algebraic result:

Lemma 3.4 *Let $Q, R \in \mathbb{C}[z]$ be coprime with $\max\{\deg Q, \deg R\} = k \geq 0$, and let $\lambda_1, \ldots, \lambda_m$ be distinct elements of $\mathbb{C}$. Then the polynomials $P_1(z), \ldots P_m(z)$, defined by*

$$(z - \lambda_i)P_i(z) = R(\lambda_i)Q(z) - Q(\lambda_i)R(z) \tag{3.32}$$

span a $\min\{k, m\}$-dimensional subspace of $\mathbb{C}_{k-1}[z]$.

Proof: Let $n = \min\{k, m\}$. Then it is enough to show that $P_1, \ldots, P_n$ are linearly independent. Assuming that $\deg Q = k$, we note that $P_i(z) = R(z)\tilde{Q}_i(z) - Q(z)\tilde{R}_i(z)$, where $\tilde{Q}_i(z) = (Q(z) - Q(\lambda_i))/(z - \lambda_i)$ and $\tilde{R}_i(z) = (R(z) - R(\lambda_i))/(z - \lambda_i)$. Suppose the P_i are linearly dependent. Then $R(z)S(z) = Q(z)T(z)$ where $S(z) = \sum_i \alpha_i\tilde{Q}_i(z)$ and $T(z) = \sum_i \alpha_i\tilde{R}_i(z)$, for some $0 \neq (\alpha_1, \ldots, \alpha_n)^T \in \mathbb{C}^n$. Because Q and R are coprime, this implies that S and T vanish identically. But one may easily show that the $\tilde{Q}_i$ are

linearly independent, by explicitly considering their coefficients. We therefore obtain a contradiction. ■

In our application, $m = |\Omega|$ with $\lambda_i = -\omega_i^2$ for each $i = 1, \ldots, m$ and $k = \max\{\deg p, \deg q\} = \mathfrak{V}$. Thus $\dim \mathcal{T}\mathrm{Ran}\, M_2 = \min\{|\Omega|, \mathfrak{V}\}$ and so

$$\dim \ker \mathcal{T} = \min\{|\Omega| - \mathfrak{V}, 0\}. \tag{3.33}$$

It follows that $\mathrm{rank}\, M_1 - \mathrm{rank}\, M_2 = \mathrm{sig}\, M_1 - \mathrm{sig}\, M_2 = \mathfrak{V} - |\Omega|$, from which (3.16) and (3.17) follow. ■

4 The GPI Hamiltonian

4.1 Locality and Spectral Properties

The results of the previous two sections allow the construction of a unitary dilation $\hat{\mathcal{T}}$ of the integral transform $\mathcal{T}$. Here, we employ $\hat{\mathcal{T}}$ to define a GPI Hamiltonian consistent with scattering theory (3.1). We denote $\Pi_r = \mathcal{H}_r \oplus \mathcal{M}_1$ and $\Pi_k = \mathcal{H}_k \oplus \mathcal{M}_2$ with J-inner products specified by $J_r = \mathbb{1}_{\mathcal{H}_r} \oplus \mathrm{sgn}\,(M_1)$, and $J_k = \mathbb{1}_{\mathcal{H}_k} \oplus \mathrm{sgn}\,(M_2)$. In terms of our general discussion in Section 2.2, we set $A = -d^2/dr^2$ on domain $C_0^\infty(0,\infty)$, and define $\mathcal{T}_+ = \mathcal{S}$, $\mathcal{T}_- = \mathcal{C}$, setting a_+ and a_- to be multiplication by $\cos\delta_0(k)$ and $\sin\delta_0(k)$ respectively. Thus $A_+ = \mathcal{S}^* k^2 \mathcal{S}$, the self-adjoint extension of A with Dirichlet boundary conditions at the origin, whilst $A_- = \mathcal{C}^* k^2 \mathcal{C}$ is the extension with Neumann boundary conditions at the origin. The operators $A_\pm + 1$ both have bounded inverse.

The S-wave GPI Hamiltonian is defined by

$$h_{\mathrm{gpi}} = \hat{\mathcal{T}}^\dagger \begin{pmatrix} k^2 & 0 \\ 0 & \Lambda \end{pmatrix} \hat{\mathcal{T}}, \tag{4.1}$$

where Λ is a $\mathrm{sgn}\,(M_2)$-self-adjoint operator $\Lambda^\dagger = \Lambda$ on $\mathcal{M}_2$. To fix Λ, we require that $h_{\mathrm{gpi}}(\psi, 0)^T = (-\psi'', 0)^T$ for all $\psi \in C_0^\infty(0,\infty)$ as a locality requirement. For general $\psi \in \mathcal{M}_2$, we have

$$A^*\psi = -\sum_{\omega\in\Omega} \alpha_\omega \omega^2 |\xi_\omega\rangle\langle\xi_{\overline{\omega}} \mid M_2^{-1}\psi\rangle, \tag{4.2}$$

so $\mathcal{M}_2$ is invariant under A^* and it follows immediately from Section 2.2 that

Theorem 4.1 *In the generic case, the unique choice of* Λ *consistent with locality is*

$$\Lambda = -\left(\mathrm{sgn}\,(M_2)|M_2|^{1/2}\right)^{-1} \sum_{\omega\in\Omega} \alpha_\omega \omega^2 |\xi_\omega\rangle\langle\xi_{\overline{\omega}}||M_2|^{-1/2}. \tag{4.3}$$

We proceed to determine the eigenvectors and eigenvalues of Λ. First note that $\langle\xi_{\overline{\omega_j}} \mid M_2^{-1}\xi_{\omega_i}\rangle = \alpha_{\omega_i}^{-1}\delta_{ij}$, which follows from the identity $\xi_{\omega_i} = \sum \alpha_\omega |\xi_\omega\rangle\langle\xi_{\overline{\omega}} \mid M_2^{-1}\xi_{\omega_i}\rangle$. It is then a matter of computation to see that $\varphi_i = \left(\mathrm{sgn}\,(M_2)|M_2|^{1/2}\right)^{-1}\xi_{\omega_i}$ is an eigenvector of Λ with eigenvalue $-\omega_i^2$ for each $i = 1, \ldots, |\Omega|$. Because Λ has rank $|\Omega|$, this exhausts the discrete spectrum of h_{gpi}. The following is then immediate.

Theorem 4.2 *In the generic case, and with Λ is defined as above, $h_{\rm gpi}$ has the following spectral properties: $\sigma(h_{\rm gpi}) = \sigma_{\rm ac}(h_{\rm gpi}) \cup \sigma_{\rm pp}(h_{\rm gpi})$ where $\sigma_{\rm ac}(h_{\rm gpi}) = \mathbb{R}^+$ and $\sigma_{\rm pp}(h_{\rm gpi})$ consists of the $|\Omega|$ eigenvalues $-\omega_i^2$, whose corresponding eigenvectors are*

$$\psi_i = \hat{\mathcal{T}}^\dagger \varphi_i = \begin{pmatrix} \xi_{\omega_i} \\ \mathcal{T}\left(\mathrm{sgn}\,(M_2)|M_2|^{1/2}\right)^{-1} \xi_{\omega_i} \end{pmatrix}. \tag{4.4}$$

The absolutely continuous subspace is the Hilbert space $\hat{\mathcal{T}}^\dagger \mathcal{H}_k$.

This bears out our earlier statement that the poles of the scattering amplitude on the physical sheet correspond to the discrete energy spectrum, if locality is imposed.

The physical Hilbert space is required to be a positive definite invariant subspace of Π_r relative to $h_{\rm gpi}$.[4] In Π_k, we have the $[\cdot,\cdot]_{\Pi_k}$-orthogonal decomposition $\Pi_k = \mathcal{H}_k[+]\mathcal{M}_2$, where $\mathcal{M}_2$ is spanned by the eigenvectors φ_i of Λ. We compute

$$[\varphi_i, \varphi_j]_{\mathcal{M}_2} = \langle \xi_{\omega_i} \mid M_2^{-1} \xi_{\omega_j} \rangle = \begin{cases} 0 & \omega_i \neq \overline{\omega_j} \\ \alpha_{\omega_j}^{-1} & \omega_i = \overline{\omega_j}. \end{cases} \tag{4.5}$$

Hence Π_k is decomposable as $\Pi_k = \mathcal{H}_k[+]E_+[+]E_-[+]H$ where E_+ is spanned by the φ_i with $[\varphi_i, \varphi_i]_{\mathcal{M}_2} > 0$ ($\alpha_{\omega_i} > 0$), E_- is spanned by those with $[\varphi_i, \varphi_i]_{\mathcal{M}_2} < 0$ ($\alpha_{\omega_i} < 0$), and H is the *hyperbolic invariant subspace* spanned by those φ_i with $\omega_i \notin \mathbb{R}$. Moreover, this is a decomposition into invariant subspaces, because $D(k^2)$ is dense in $\mathcal{H}_k$. The physical Hilbert space $\mathcal{H}_{\rm phys}$ is therefore defined by

$$\mathcal{H}_{\rm phys} = \hat{\mathcal{T}}^\dagger(\mathcal{H}_k[+]E_+). \tag{4.6}$$

We briefly discuss the uniqueness of the GPI Hamiltonian constructed in this way. As noted in Section 2.1, $\hat{\mathcal{T}}$ is unique up to further unitary dilation and unitary equivalence because the M_i are of finite rank. Further dilation merely corresponds to the (trivial) freedom to form the direct sum of $h_{\rm gpi}$ with the Hamiltonian of an arbitrary independent system. On the other hand, replacing $\hat{\mathcal{T}}$ by $(\mathbb{1} \oplus U_2)\hat{\mathcal{T}}(\mathbb{1} \oplus U_1)$ where U_i is a $\mathrm{sgn}\, M_i$-unitary operator on $\mathcal{M}_i$ for $i = 1, 2$, it is easy to show that the local GPI Hamiltonian $h'_{\rm gpi}$ obtained is given by

$$h'_{\rm gpi} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & U_1 \end{pmatrix}^\dagger h_{\rm gpi} \begin{pmatrix} \mathbb{1} & 0 \\ 0 & U_1 \end{pmatrix}. \tag{4.7}$$

We have therefore constructed a family of unitarily equivalent GPI Hamiltonians on Π_r corresponding to the same scattering data. It is clearly sufficient to study $h_{\rm gpi}$ alone in order to determine the domain and scattering properties of $h'_{\rm gpi}$.

[4] An invariant subspace $\mathcal{L}$ of a J-space $\mathcal{K}$ relative to a linear operator A on $\mathcal{K}$ is a subspace of $\mathcal{K}$ such that $\overline{D(A) \cap \mathcal{L}} = \mathcal{L}$ and $\mathrm{Ran}\, A|_{\mathcal{L}} \subset \mathcal{L}$, where the closure is taken in the norm topology of $\mathcal{K}$.

4.2 Domain and Resolvent

We now determine the domain and explicit action of the operator $h_{\rm gpi}$ under the locality assumption. Our result is the following:

Theorem 4.3 *Let* $\Theta_0 = (2/\pi)^{1/2} k^{2\mathfrak{v}-1}(p(k^2)^2 + k^2 q(k^2)^2)^{-1/2}$. *Then in the generic case,*

$$D(h_{\rm gpi}) = \left\{ \begin{pmatrix} \varphi \\ \Phi \end{pmatrix} \mid \varphi, \varphi' \in AC_{\rm loc}(0,\infty),\ \varphi, \varphi'' \in L^2; \quad \Phi \in \mathcal{M}_1, \right.$$
$$\left. \Theta - \lambda[\varphi]\Theta_0 \in D(k^2) \cap \mathcal{M}_1 \right\}, \tag{4.8}$$

where $\Theta = \operatorname{sgn} M_1 |M_1|^{1/2}\Phi$ *and*

$$\lambda[\varphi] = \begin{cases} P\varphi(0) & \deg p > \deg q \\ P\varphi(0) - Q\varphi'(0) & \deg p = \deg q \\ -Q\varphi'(0) & \deg p < \deg q, \end{cases} \tag{4.9}$$

and P *and* Q *are the leading coefficients of* $p(z)$ *and* $q(z)$ *respectively. (In the case* $M_1 = 0$, $D(h_{\rm gpi}) = \{\varphi \mid \varphi, \varphi' \in AC_{\rm loc}(0,\infty),\ \varphi, \varphi'' \in L^2;\ \lambda[\varphi] = 0\}$.*) Moreover,*

$$h_{\rm gpi} \begin{pmatrix} \varphi \\ \Phi \end{pmatrix} = \begin{pmatrix} -\varphi'' \\ \tilde{\Phi} \end{pmatrix}, \tag{4.10}$$

where $\tilde{\Phi}$ *is given in terms of* $\tilde{\Theta} = \operatorname{sgn} M_1 |M_1|^{1/2}\tilde{\Phi}$ *by*

$$\tilde{\Theta} = k^2(\Theta - \lambda[\varphi]\Theta_0) + \left(\frac{2}{\pi}\right)^{1/2} \frac{k(\lambda[\varphi]k^{2\mathfrak{v}} - \varphi(0)p(k^2) + \varphi'(0)q(k^2))}{(p(k^2)^2 + k^2 q(k^2)^2)^{1/2}}. \tag{4.11}$$

Proof: The result is a direct application of the discussion in Section 2.2. The key point is that, for each $\varphi \in D(-d^2/dr^2|^*_{C_0^\infty(0,\infty)})$, the vectors χ_+ and χ_- are given by

$$\chi_+ = -\varphi(0)e^{-r} \qquad \text{and} \qquad \chi_- = \varphi'(0)e^{-r}, \tag{4.12}$$

which follows because χ_+ (χ_-) is the unique element of $\ker(-d^2/dr^2|^*_{C_0^\infty(0,\infty)} + 1)$ such that $\varphi + \chi_+$ ($\varphi + \chi_-$) is in the domain of the Laplacian with Dirichlet (Neumann) boundary conditions at the origin. ■

The resolvent of $h_{\rm gpi}$ may be written in the form of Krein's formula as

$$(h_{\rm gpi} - z)^{-1} = \begin{pmatrix} R_0(z) & 0 \\ 0 & R_1(z) \end{pmatrix} + \frac{q(z)}{p(z) + (-z)^{1/2} q(z)} F(z) F(\overline{z})^\dagger. \tag{4.13}$$

Here, $R_0(z) = \mathcal{S}^{-1}(k^2 - z)^{-1}\mathcal{S}$ is the free resolvent and the defect element $F(z) \in \Pi_r$ is given by

$$F(z) = \begin{pmatrix} e^{-(-z)^{1/2} r} \\ (\operatorname{sgn} M_1 |M_1|^{1/2})^{-1} \Psi(z) \end{pmatrix}, \tag{4.14}$$

where $\Psi(z) \in \mathcal{M}_1$ is

$$\Psi(z) = \left(\frac{2}{\pi}\right)^{1/2} \frac{k(p(k^2)q(z) - p(z)q(k^2))}{(k^2 - z)(p(k^2)^2 + k^2 q(k^2)^2)^{1/2}}, \tag{4.15}$$

and the operator $R_1(z)$ is defined on $\mathcal{M}_1$ by

$$R_1(z)\Phi = (\operatorname{sgn} M_1 |M_1|^{1/2})^{-1} \left(\frac{2}{\pi}\right)^{1/2} \frac{k(Q(k^2) - Q(z)q(k^2)/q(z))}{(k^2 - z)(p(k^2)^2 + k^2 q(k^2)^2)^{1/2}}, \tag{4.16}$$

where $Q(z)$ is defined in terms of Φ by

$$\Theta = \operatorname{sgn} M_1 |M_1|^{1/2}\Phi = \left(\frac{2}{\pi}\right)^{1/2} \frac{kQ(k^2)}{(p(k^2)^2 + k^2 q(k^2)^2)^{1/2}}. \tag{4.17}$$

The above expression for $R(z)$ may be verified directly using Theorem 4.3, and the fact that

$$[(\operatorname{sgn} M_1 |M_1|^{1/2})^{-1}\Psi(\overline{z}), \Phi]_{\mathcal{M}_1} = -\frac{Q(z)}{q(z)}, \tag{4.18}$$

which is required when one takes inner products with $F(\overline{z})$. Using this result, it follows that (4.13) holds for elements of form $(0, \Phi)^T$ with $Q(z) = 0$; direct computation establishes it for $Q(z) \equiv 1$ and also for vectors of form $(\varphi, 0)^T$ with $\varphi \in \mathcal{H}_r$.[5] Thus (4.13) holds on the whole of Π_r. It remains to establish equation (4.18). Multiplying through by $q(z)$, the LHS of (4.18) is equal to

$$\langle q(\overline{z})\Psi(\overline{z}) \mid M_1^{-1}\Theta\rangle = \langle \mathcal{T}^* q(\overline{z})\Psi(\overline{z}) \mid M_2^{-1}\mathcal{T}^*\Theta\rangle + \langle q(\overline{z})\Psi(\overline{z}) \mid \Theta\rangle. \tag{4.19}$$

Using the identity $\langle \xi_{\overline{\omega_j}} \mid M_2^{-1}\xi_{\omega_i}\rangle = \alpha_{\omega_i}^{-1}\delta_{ij}$ and the results of Section 3, the first term is

$$\langle \mathcal{T}^* q(\overline{z})\Psi(\overline{z}) \mid M_2^{-1}\mathcal{T}^*\Theta\rangle = \sum_{\omega\in\Omega} \frac{p(z) - \omega q(z)}{q(-\omega^2)(\omega^2 + z)} Q(-\omega^2)\alpha_\omega. \tag{4.20}$$

The required result then follows from the calculation

$$\begin{aligned} \langle q(\overline{z})\Psi(\overline{z}) \mid \Theta\rangle &= \frac{1}{\pi}\int_{-\infty}^{\infty} dk \frac{ikQ(k^2)(p(z) - ikq(z))}{(k^2 - z)(p(k^2) - ikq(k^2))} \\ &= -Q(z) - \sum_{\omega\in\Omega} \frac{p(z) - \omega q(z)}{q(-\omega^2)(\omega^2 + z)} Q(-\omega^2)\alpha_\omega. \end{aligned} \tag{4.21}$$

4.3 Scattering Theory

In this section, we construct Møller wave operators for h_{gpi} relative to the free Hamiltonian $h_0 = \mathcal{S}^{-1}k^2\mathcal{S}$ on $\mathcal{H}_r$ in order to check that h_{gpi} actually exhibits the required scattering behaviour. Because scattering is a function of the continuous spectrum only,

[5] Here, it is useful to employ the decomposition $\mathcal{H}_r = \overline{\operatorname{Ran}(-d^2/dr^2 - z)|_{C_0^\infty(0,\infty)}} \oplus \mathbb{C}e^{-(-\overline{z})^{1/2}r}$.

our results in this section are actually independent of the precise form of Λ, and therefore of the locality requirement.

We work in the S-wave, and employ a two space setting: let B be self-adjoint on $\mathcal{H}_1$, A be self-adjoint on $\mathcal{H}_2$ and $\mathcal{J}$ be a bounded operator from $\mathcal{H}_1$ to $\mathcal{H}_2$. Then the Møller operators $\Omega^{\pm}(A, B; \mathcal{J})$ are defined by

$$\Omega^{\pm}(A, B; \mathcal{J}) = \lim_{t \to \mp\infty} e^{iAt} \mathcal{J} e^{-iBt} P_{\rm ac}(B), \tag{4.22}$$

and are said to be complete if the closure of $\mathrm{Ran}\Omega^{\pm}(A, B; \mathcal{J})$ is equal to $\mathrm{Ran}P_{\rm ac}(A)$.

In the following, $\mathcal{J}_r$ and $\mathcal{J}_k$ are the natural embeddings of $\mathcal{H}_r$ and $\mathcal{H}_k$ into Π_r and Π_k respectively.

Theorem 4.4 *Let $\mathcal{J} : \mathcal{H}_r \to \Pi_r$ be given by $\mathcal{J} = \hat{\mathcal{T}}^\dagger \mathcal{J}_k \mathcal{T}$. Then $\Omega^{\pm}(h_{\rm gpi}, h_0; \mathcal{J})$ exist, are complete, and given by*

$$\Omega^{\pm}(h_{\rm gpi}, h_0; \mathcal{J}) = \hat{\mathcal{T}}^\dagger \mathcal{J}_k e^{\pm i\delta_0(k)} \mathcal{S}, \tag{4.23}$$

where $\delta_0(k)$ is given by (3.1).

Proof: Writing U_t for multiplication by $e^{-ik^2 t}$ on $\mathcal{H}_k$, we have

$$\begin{aligned} e^{ih_{\rm gpi}t} \mathcal{J} e^{-ih_0 t} P_{\rm ac}(h_0) &= \hat{\mathcal{T}}^\dagger \begin{pmatrix} U_{-t} & 0 \\ 0 & \exp i\Lambda t \end{pmatrix} \hat{\mathcal{T}} \mathcal{J} \mathcal{S}^{-1} U_t \mathcal{S} \\ &= \hat{\mathcal{T}}^\dagger \mathcal{J}_k U_{-t} \mathcal{T} \mathcal{S}^{-1} U_t \mathcal{S}. \end{aligned} \tag{4.24}$$

Now, for any $u(k) \in C_0^\infty(0, \infty)$,

$$\begin{aligned} \|U_{-t} \mathcal{T} \mathcal{S}^{-1} U_t u(k) - e^{\pm i\delta_0(k)} u(k)\|^2 &= \|\sin\delta_0(k) \mathcal{C}(\mathcal{C}^{-1} \pm i\mathcal{S}^{-1}) U_t u(k)\|^2 \\ &\leq \frac{2}{\pi} \int_0^\infty dr \left| \int_0^\infty dk e^{i(\pm kr - k^2 t)} u(k) \right|^2, \end{aligned} \tag{4.25}$$

which vanishes as $t \to \mp\infty$ by (non)-stationary phase arguments (see the Corollary to Theorem XI.14 in [26]). Thus $U_{-t} \mathcal{T} \mathcal{S}^{-1} U_t \to e^{\pm i\delta_0(k)}$ strongly as $t \to \mp\infty$. The existence and form of the Møller operators are then immediate. One easily checks that they are unitary maps from $\mathcal{H}_r$ to $P_{\rm ac}(h_{\rm gpi}) = \hat{\mathcal{T}}^\dagger \mathcal{J}_k \mathcal{H}_k$, to establish completeness. ■

We conclude that our construction does indeed yield the required scattering theory, and also that – as a by-product of the construction – complete Møller operators may easily and explicitly be determined.

5 Examples

As an application, we construct the class of GPI models with scattering data

$$\cot\delta_0(k) = -\frac{1}{kL} + kM, \tag{5.1}$$

where L is the scattering length, and M is twice the effective range. These models therefore represent the effective range approximation to the behaviour of a non-point interaction in the S-wave. This class of models has been partially studied by Shondin [11], who considered the case $M < 0$ ('models of type B_2') and also appears as a special case of the models considered by Pavlov in [8]. (We also note that van Diejen and Tip [13] have constructed models of type $\cot\delta_0(k) = (ak + bk^3 + ck^5)^{-1}$ using the distributional method.) The case $M > 0$ does not appear to have been treated before. Our construction provides a unified construction for all models in the above class, and also provides the spectral representation such models as a by-product of the construction (although we will not state this explicitly).

The above class of GPI models contains two interesting sub-families: the ordinary point interactions ($M = 0$) and also the resonance point interactions arising formally by setting $L = \infty$, i.e., $\cot\delta_0(k) = kM$ with $M \in \mathbb{R} \cup \{\infty\}$. Such models are required in situations where the scattering length is generically forced to be infinite, for example in certain systems of supersymmetric quantum mechanics.

We begin by briefly treating the point interactions, both for completeness and also to demonstrate how this class arises in our formalism. We then turn to the general case, obtaining RPI models in the limit $L \to -\infty$.

5.1 Point Interactions

The required integral transform is

$$\mathcal{T} = (1 + (kL)^2)^{-1/2}\mathcal{S} - kL(1 + (kL)^2)^{-1/2}\mathcal{C}. \tag{5.2}$$

In the cases $L = 0, \infty$, $\mathcal{T}$ reduces to $\mathcal{S}$ and $\mathcal{C}$ respectively, and the Hamiltonian is given immediately by $\mathcal{T}^*k^2\mathcal{T}$. We exclude these cases from the rest of our discussion.

We therefore apply the construction of Section 3, with $p(z) \equiv -L^{-1}$ and $q(z) \equiv 1$. We find that $\mho = 0$, so $M_1 = 0$ (i.e., $\mathcal{T}\mathcal{T}^* = \mathbb{1}$). Straightforward application of Proposition 3.1 yields

$$M_2 = \begin{cases} |\chi_L\rangle\langle\chi_L| & L > 0 \\ 0 & L < 0, \end{cases} \tag{5.3}$$

where $\chi_L(r) = (2/L)^{1/2}e^{-r/L}$ is normalised to unity. Hence if $L < 0$, $\mathcal{T}$ is unitary and the Hamiltonian is $h_L = \mathcal{T}^*k^2\mathcal{T}$, with purely absolutely continuous spectrum $\mathbb{R}^+$. In the case $L > 0$, the momentum Hilbert space is extended to $\mathcal{H}_k \oplus \mathbb{C}$, representing a single bound state, and the unitary dilation $\hat{\mathcal{T}} : \mathcal{H}_r \to \mathcal{H}_k \oplus \mathbb{C}$ takes form

$$\hat{\mathcal{T}} = \begin{pmatrix} \mathcal{T} \\ \langle\chi_L| \end{pmatrix}; \qquad \hat{\mathcal{T}}^* = \begin{pmatrix} T^* & |\chi_L\rangle \end{pmatrix}. \tag{5.4}$$

($\mathcal{H}_k \oplus \mathbb{C}$ has the obvious inner product.) The Hamiltonian is

$$h_L = \hat{\mathcal{T}}^{-1} \begin{pmatrix} k^2 & 0 \\ 0 & \lambda \end{pmatrix} \hat{\mathcal{T}} = \mathcal{T}^*k^2\mathcal{T} + \lambda|\chi_L\rangle\langle\chi_L|, \tag{5.5}$$

and the locality requirement fixes $\lambda = -L^{-2}$, which is, of course, the usual value. Finally, the domain of h_L is given by Theorem 4.3 as the space of φ with $\varphi, \varphi' \in AC_{\rm loc}(0,\infty)$, $\varphi'' \in L^2$ and satisfying the well known boundary condition

$$\varphi(0) + L\varphi'(0) = 0. \tag{5.6}$$

To summarise, all the well known properties of point interactions may be derived within our formalism.

5.2 Effective Range Approximation

In this section, we maintain $M \neq 0$, $L \neq 0$, setting $p(z) = -L^{-1} + zM$ and $q(z) \equiv 1$. We will not explicitly construct the dilation (although this follows immediately from our discussion), but will use the results of Section 4 to read off the domain and action of the GPI Hamiltonian $h_{L,M}$.

Using the results of Section 3, we find

$$\mho = 1; \qquad |\Omega| = \begin{cases} 1 + \frac{1}{2}(\operatorname{sgn} M + \operatorname{sgn} L) & L \neq \infty \\ \frac{1}{2}(1 + \operatorname{sgn} M) & L = \infty. \end{cases} \tag{5.7}$$

Writing $W(z) = -M(z-\omega_1)(z-\omega_2)$, Ω is the subset of $\{\omega_1, \omega_2\}$ lying in the left-hand half-plane, and we have $\omega_1 + \omega_2 = -M^{-1}$, $\omega_1\omega_2 = (ML)^{-1}$. The residues α_ω are

$$\alpha_{\omega_1} = -\frac{2\omega_1}{M(\omega_1 - \omega_2)}, \qquad \alpha_{\omega_2} = \frac{2\omega_2}{M(\omega_1 - \omega_2)}. \tag{5.8}$$

In addition, the space $\mathcal{M}_1 = \operatorname{Ran} M_1$ is equal to $\mathbb{C}|\eta\rangle$, where

$$\eta(k) = \mathcal{N}\frac{k}{(k^2 + (k^2M - L^{-1})^2)^{1/2}}, \tag{5.9}$$

and the normalisation constant is

$$\mathcal{N} = \begin{cases} (2|M|/\pi)^{1/2} & ML > 0 \\ (2|M|/\pi)^{1/2}(1 - 4ML^{-1})^{1/4} & ML < 0. \end{cases} \tag{5.10}$$

Using Proposition 3.2, we obtain

$$M_1 = \lambda|\eta\rangle\langle\eta|; \qquad \lambda = \begin{cases} +1 & M < 0, L < 0 \\ -\operatorname{sgn} M(1 - 4ML^{-1})^{-1/2} & ML < 0 \\ -1 & M > 0, L > 0. \end{cases} \tag{5.11}$$

Accordingly, the extended position inner product space is $\Pi_r = \mathcal{H}_r \oplus \mathbb{C}$ with J-inner product specified by $J = \mathbb{1} \oplus (-\operatorname{sgn} M)$. The scalar component is the coefficient of $|\eta\rangle$

in $\mathcal{M}_1$. For all generic cases (i.e., all cases other than $L = 4M > 0$) Theorem 4.3 entails that the domain of $h_{L,M}$ is

$$D(h_{L,M}) = \left\{ \begin{pmatrix} \varphi \\ \Phi \end{pmatrix} \mid \varphi, \varphi' \in AC_{\mathrm{loc}}(0,\infty),\ \varphi, \varphi'' \in L^2; \quad \Phi = -|M|^{1/2}\varphi(0) \right\}, \quad (5.12)$$

and that the action is

$$h_{L,M} \begin{pmatrix} \varphi \\ -|M|^{1/2}\varphi(0) \end{pmatrix} = \begin{pmatrix} -\varphi'' \\ -\operatorname{sgn} M |M|^{-1/2}(\varphi'(0) + L^{-1}\varphi(0)) \end{pmatrix}. \quad (5.13)$$

Moreover, one may show that these equations also hold in the non-generic case $L = 4M > 0$.

It is worth noting how this domain and action correspond to the scattering data (5.1). Solving the equation $h_{L,M}(\varphi, \Phi)^T = k^2(\varphi, \Phi)^T$ for the generalised eigenfunctions of $h_{L,M}$, we find $\varphi(r) \propto \sin(kr + d(k))$ for some $d(k)$, and also obtain the relation

$$-\operatorname{sgn} M |M|^{-1/2}(\varphi'(0) + L^{-1}\varphi(0)) = -k^2|M|^{1/2}\varphi(0), \quad (5.14)$$

which entails that $k \cot d(k) = \varphi'(0)/\varphi(0) = -L^{-1} + k^2 M$. Thus $d(k)$ is precisely the scattering data $\delta_0(k)$.

The RPI models, which have scattering data $\cot \delta_0(k) = kM$ are obtained in the same way. The space $\mathcal{M}_1$ is spanned by $\psi_M(k) = (2|M|/\pi)^{1/2}(1 + (kM)^2)^{-1/2}$, and the operator M_1 is found to be $M_1 = -(\operatorname{sgn} M)|\psi_M\rangle\langle\psi_M|$. Thus the inner product space is $\Pi_r = \mathcal{H}_r \oplus \mathbb{C}$ with $J = \mathbb{1} \oplus (-\operatorname{sgn} M)$. They have the domain (5.12) and action

$$h_{\mathrm{rpi},M} \begin{pmatrix} \varphi \\ -|M|^{1/2}\varphi(0) \end{pmatrix} = \begin{pmatrix} -\varphi'' \\ -\operatorname{sgn} M |M|^{-1/2}\varphi'(0) \end{pmatrix}. \quad (5.15)$$

Let us consider the physical Hilbert space for these models. From Section 4, this is constructed by projecting out the hyperbolic invariant subspace, and also those eigenfunctions with negative norm squared (if present). The bound states of $h_{L,M}$ are clearly vectors of form $(\xi_\omega, |M|^{1/2})^T$ with norm squared equal to $-(2\mathrm{Re}\,\omega)^{-1} - M$, where ω is a root of $\omega^2 + M^{-1}\omega + (ML)^{-1} = 0$. There are four cases to consider:

Case (i): $M < 0$. Π_r is positive definite so no projection is required.

Case (ii): $M > 0$, $L < 0$. There is a unique bound state with

$$\omega = \frac{1 + (1 - 4M/L)^{1/2}}{-2M} \quad (5.16)$$

and negative norm squared. Projecting this state out, we obtain

$$\mathcal{H}_{\mathrm{phys}} = \left\{ \begin{pmatrix} \varphi \\ M^{-1/2}\langle \xi_\omega \mid \varphi \rangle \end{pmatrix} \mid \varphi \in \mathcal{H}_r \right\}. \quad (5.17)$$

Case (iii): $M > 0$, $0 < L < 4M$. There are two bound states with complex conjugate eigenvalues. Accordingly, their eigenfunctions span a hyperbolic invariant subspace. Projecting this subspace out, we find

$$\mathcal{H}_{\rm phys} = \left\{ \begin{pmatrix} \varphi \\ M^{-1/2}\langle \frac{1}{2}(\xi_\omega + \xi_{\overline{\omega}}) \mid \varphi \rangle \end{pmatrix} \mid \varphi \in \mathcal{H}_r \text{ s.t. } \langle (\xi_\omega - \xi_{\overline{\omega}}) \mid \varphi \rangle = 0 \right\}, \tag{5.18}$$

where ω is given by equation (5.16).

Case (iv): $M > 0$, $L > 4M$. There are two bound states with real eigenvalues. However, only the state specified by (5.16) has negative norm. Projecting this out, we arrive at the same expression for $\mathcal{H}_{\rm phys}$ as in case (ii).

RPI models are covered by Case (i) for $M < 0$, and have $\mathcal{H}_{\rm phys}$ given by (5.17) for $M > 0$, with $\omega = -1/M$.

The GPI Hamiltonian acts on $\mathcal{H}_{\rm phys}$ by restriction. For example, in case (ii) above, we have

$$\begin{aligned} D(h_{L,M}|_{\mathcal{H}_{\rm phys}}) \;=\; \Bigg\{ & \begin{pmatrix} \varphi \\ M^{-1/2}\langle \xi_\omega \mid \varphi \rangle \end{pmatrix} \mid \varphi, \varphi' \in AC_{\rm loc}(0,\infty),\ \varphi, \varphi'' \in L^2; \\ & M\varphi(0) = -\langle \xi_\omega \mid \varphi \rangle \Bigg\} \end{aligned} \tag{5.19}$$

on which $h_{L,M}|_{\mathcal{H}_{\rm phys}}$ acts as before. The restricted operator has the same continuum spectrum as $h_{L,M}$, but has no bound states in this case. Moreover, the property of locality is partially lost: it is clear that vectors of form $(\varphi, 0)^T$ with $\varphi \in C_0^\infty(0,\infty)$ are in $\mathcal{H}_{\rm phys}$ only if $\varphi \perp \xi_\omega$. However, for elements of this form in $\mathcal{H}_{\rm phys}$, it remains the case that $h_{L,M}|_{\mathcal{H}_{\rm phys}}(\varphi, 0)^T = (-\varphi'', 0)^T$. Thus the properties of locality and 'positivity' are not entirely compatible.

5.3 Physical Interpretation

In this section, we discuss how the effective range models constructed above may be used to model Schrödinger operators $H = -\triangle + V$, where V is smooth, spherically symmetric and compactly supported within radius a of the origin. Our methodology extends that described in [3], in which the scattering length approximation is discussed.

Given a smooth spherically symmetric potential $V(r)$ supported within radius a of the origin, we may find the 'best fit' GPI model $h_{L,M}$ as follows. Let u_0 be the S-wave zero energy eigenfunction, i.e., the solution to $-u_0'' + Vu_0 = 0$ with regular boundary conditions at the origin. Then the arguments of Section 11.2 of [17] give the low energy parameters L and M as

$$L = a - \left. \frac{u_0}{u_0'} \right|_{r=a}; \tag{5.20}$$

and

$$M = a\left\{1 - \frac{a}{L} + \frac{1}{3}\left(\frac{a}{L}\right)^2 - \left(1 - \frac{a}{L}\right)^2 \frac{\int_0^a |u_0(r)|^2 dr}{a|u_0(a)|^2}\right\}. \tag{5.21}$$

Thus the scattering behaviour is $\cot\delta_0(k) = -(kL)^{-1} + kM + O(k^3)$ and the best fit GPI model in our class is $h_{L,M}$. We refer to equations (5.20) and (5.21) as *fitting formulae*; equation (5.20) is the fitting formula employed in [3]. The range of energies for which the approximation is valid can be determined by a 'believability' analysis analogous to that described in [3]. We will not do this here.

Note that M obeys the bound

$$-\infty \leq M < a\left\{1 - \frac{a}{L} + \frac{1}{3}\left(\frac{a}{L}\right)^2\right\}. \tag{5.22}$$

Moreover, this bound is best possible: for any $L \in \mathbb{R} \cup \{\infty\}$ and any M in the above range, one can clearly find a smooth function $u_0(r)$ satisfying regular boundary conditions at the origin, $u_0 \propto (1 - r/L)$ for $r > a$ and such that (5.21) holds. Then the potential defined by $V(r) = u_0''(r)/u_0(r)$ has S-wave scattering behaviour approximated to second order by $h_{L,M}$. The contribution to the total scattering cross section from the effective range term generally outweighs that from higher angular momenta, so the S-wave GPI model provides a second order approximation to the full scattering behaviour.

Finally, we discuss the interpretation of the discrete spectrum of $h_{L,M}$. We have constructed $h_{L,M}$ so that its scattering behaviour matches that of a given Schrödinger operator at low energies, E. For larger $|E|$, the approximation breaks down – in the language of [3] we say that it is no longer 'believable'. Thus, deeply bound states are unlikely to be believable. In particular, for $0 < L < 4M$, $h_{L,M}$ exhibits a complex conjugate pair of eigenvalues, which can never be believable.[6] Such phenomena are artifacts of the idealisation process, due to the truncation of the low energy expansion. The issue of believability is discussed in [3]; similar comments are made in [13].

6 Conclusion

We begin by discussing various generalisations of our method. There are many situations in which the analysis of Section 2.2 may be applied. In two dimensions, for example, one can consider radial GPI Hamiltonians which agree with

$$h = -\frac{1}{r}\frac{d}{dr}r\frac{d}{dr} + \frac{\nu^2}{r^2} \tag{6.1}$$

away from the origin, as models for an infinitesimal 'dot' of magnetic flux ν, with $|\nu| < 1$. In this case, one must employ Hankel transforms rather than sine and cosine transforms.

[6] These are not eigenvalues of $h_{L,M}$ restricted to the physical Hilbert space. However, they persist as poles in the scattering amplitude and our remarks still apply: $h_{L,M}$ does not give a reliable approximation to the scattering theory at those scales.

In [19] we will implement this programme to construct a models of RPI type for the Dirac equation in the presence of an infinitesimal tube of flux. These models provide the leading order approximation to the scattering data.

Our method could also be applied to S-wave GPI models with a Coulombic tail. In this case, the appropriate integral transforms would be based upon Whittaker functions and the scattering data would be specified in terms of Coulomb-modified partial wave shifts. In this case, the dimension of $\mathcal{M}_2$ would be countably infinite, due to the countable discrete spectrum of such models. However, one would expect $\mathcal{M}_1$ to remain finite dimensional for simple models.

Secondly, it is of interest to generalise the unitary dilation method to sectors of higher angular momentum with $\ell \geq 1$ (and the corresponding analogues for magnetic flux dots – i.e., $|\nu| \geq 1$ – and Coulombic GPI for $\ell \geq 1$). This is more problematic, because the radial Hamiltonian $-d^2/dr^2 + \ell(\ell+1)/r^2$ is essentially self-adjoint on $C_0^\infty(0,\infty)$ and so the method of Section 2.2 does not apply. Here, it might be possible to obtain a suitable integral transform by analysing the distributional construction. We hope to return to this elsewhere.

Finally, we consider applications to the definition of arrays of point scatterers. Here, the most likely use of our methods is to generate the 'monomer' by inverse scattering. By passing to the resolvent written in the form of Krein's formula, one can isolate the appropriate 'defect element' and proceed to form the array by methods discussed in [13], which generalise the procedure for arrays of PI developed in [27].

To summarise, we have introduced an inverse scattering construction for GPI models using the theory of unitary dilations, and developed the method in detail for the class of single centre S-wave GPI models with rational S-matrices. A physical locality requirement completes the specification of the Hamiltonian, whose scattering, spectral and domain properties are explicitly determined from our results.

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